Theoretical Study of a Perfectly Volatile Particle Triple Flame

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Abstract—The structure of triple flame propagating in combustible systems, containing uniformly distributed volatile fuel particles is analyzed. It is presumed that the fuel particles vaporize first to yield a gaseous fuel of known chemical structure, which is subsequently oxidized by oxidizer stream in the gas phase. The analysis is carried for a single irreversible reaction with asymptotic limit, where the value of Zeldovich number, based on the gas-phase oxidation of the gaseous fuel is large. The analysis using the unit Lewis number yields analytical result for triple flame temperature field.

I. INTRODUCTION

The importance of triple flames is now well established, in applications involving combustion phenomena, such as flame spread over solid or liquid fuel surfaces, flame propagation in mixing layers, dynamic extinction of diffusion flames, and flame stabilization in reactive streams. Early experimental observation of this structure was made by Phillips [1] and an early analytical description appears in Ohki and Tsuge [2]. Detailed analysis of triple flames and their propagation regimes was undertaken by Dold and collaborators [3,4]. Several aspects of the problem have since been investigated, including the effect of gas expansion, the influence of non-unit Lewis numbers and the stability of triple flames (see Refs. [5–9]).

The aim of this work is to extend current knowledge of triple flames by taking into account the influence of vaporization term for the fuel particles. This aspect of the problem seems to have received no attention. The aim of this paper is to investigate how triple flames, and their propagation regimes, are affected by vaporization term of perfectly volatile fuel particle in this configuration.

The paper is structured as follows: the problem is first formulated as one-step combustion process with constant density and constant conductivity properties as well as equal ratio of mass diffusivity on temperature diffusivity (unit Lewis number). The basic equations will be solved in term of non-dimensionless variables with specified non-dimensionless boundary conditions.

II. PROBLEM FORMULATION

The problem addressed herein is the steady propagation of a non premixed flame consisting of uniformly distributed volatile fuel particles. All external forces including gravitational effects are assumed to be negligible.

Other approximations introduced are that diffusion caused by pressure gradient as well as heat transport by radiation are negligible. The combustion process is modeled by a single, irreversible, one-step reaction of the form \( v_F F + v_X X \rightarrow v_P P \). Where \( v_F \) molecules of a fuel (molecular mass \( m_F \)) react with \( v_X \) molecules of an oxidizer (molecular mass \( m_X \)) to form \( v_P \) product molecules (molecular mass \( m_P \)). In the analysis it is presumed that the fuel particles vaporize to form a known gaseous compound which is then oxidized and products are assumed to be in the gaseous phase. Finally we will only consider the case of unity Lewis number that is the rate of the temperature diffusivity and the mass diffusivity of the two species are the same.

A. Basic Equations

The kinetic of vaporization are presumed to be represented by the expression

\[
W_v = Bn_r (4\pi r^2) T^n
\]  

(1)

where \( W_v \) is the mass of gaseous fuel vaporized per unit volume per second. The quantities \( B \) and \( n \) are constants which presumed to be known, and \( T \) denotes the gas temperature. For simplicity it is assumed that the particle temperature is approximately equal to the gas temperature.

The time evolution of the mass fractions of the two reactants, \( Y_F \) (the fuel mass fraction) and \( Y_X \) (the oxidizer mass fraction) is described by

\[
\rho \frac{DY_r}{Dt} = D_r \nabla^2 Y_r - v_r m_r \omega + W_v,
\]  

(2)
where \( i=F \) or \( X \), \( \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \) is the material derivative, \( \rho \) and \( \mathbf{u} \) are the fluid density and velocity, \( \omega \) is the rate of reaction in unit volume per unit time, \( W_r \) is vaporization term described by (1), and \( D_i \) is the mass diffusivity of the species \( i \). The time evolution of the temperature \( T \), is described by

\[
\frac{\rho c_p}{\rho_o} \frac{DT}{Dt} = D_T \nabla^2 T + Q\omega - W_r Q_r, \tag{3}
\]

where \( c_p \) is the specific heat at constant pressure referred to unit mass of gas, \( Q \) is the amount of heat released per reaction, \( D_T \) is the thermal conductivity and \( Q_r \) is the heat associated with vaporizing unit mass of the fuel. The Lewis numbers will be assumed unity, so

\[
\frac{D_F}{\rho_o} = \frac{D_X}{\rho_o} = \frac{D_T}{\rho_o c_p} = k, \tag{4}
\]

where \( \rho_o \) is the density of un-burnt gas far upstream which assumed constant. Therefore (2) and (3) become

\[
\rho \frac{DY}{Dt} = k \rho_o c_p \nabla^2 Y_F - v_m \omega + W_r, \tag{5}
\]

\[
\rho \frac{DY}{Dt} = k \rho_o c_p \nabla^2 Y_F - v_m \omega + W_r, \tag{6}
\]

For the reaction rate, the well known Arrhenius law will be applied by

\[
\omega = A \rho_0^{\nu_0+\nu_F} Y_F^{\nu_F} Y_X^{\nu_X} \exp(-T_a/T). \tag{7}
\]

where \( T_a \) is the activation temperature which is constant for a given reaction and the exponential factor \( A \) is approximately assumed constant and haven't temperature dependence.

We consider the problem as a uniform flow along x-axis between \( x=(-L,+L) \), by \( U_o,x \), where \( U_o \) is the propagation speed of the triple flame far upstream. We assume that the fuel mass fraction varies from \( Y_F=1 \) in fuel stream \( (y\rightarrow+L) \) to \( Y_F=0 \) in oxidizer stream \( (y\rightarrow-L) \). Similarly, the oxidizer mass fraction varies from \( Y_X=1 \) in oxidizer stream \( (y\rightarrow-L) \) to \( Y_X=0 \) in fuel stream \( (y\rightarrow+L) \) such that for upstream

\[
Y_F(-L,y) + Y_X(-L,y) = 1. \tag{8}
\]

The fuel and oxidizer are assumed to be at the same constant temperature far upstream, \( T=T_o \). Therefore the boundary conditions in a limited domain are \( T(-L,y)=T_o; \ T(0,y)=T_o \); and \( T_o(x,0)=0 \).

The fuel mixture fraction, \( Z \), is then defined as

\[
Z = \frac{r Y_F - Y_X + 1}{1+r}, \tag{9}
\]

Where \( r=v_m m_F/v_mE \). Clearly, \( Z=1 \) in the fuel stream, \( Z=0 \) in the oxidizer stream and \( Z=Z_s=1/(1+r) \) under stoichiometric condition.

It follows from (5) and (9) that \( Z \) evolves as a passive scalar:

\[
\rho \frac{DZ}{Dt} = k \rho_o c_p \nabla^2 Z. \tag{10}
\]

By eliminating the source terms as well as vaporization terms from (5) and (6), it can be shown that the specific enthalpy, which is defined below by (11) also evolve as a passive scalar (See Equation (12)):

\[
H_i = T + \frac{Q Y_i}{v_m c_p}, \tag{11}
\]

\[
\rho \frac{DH_i}{Dt} = k \rho_o c_p \nabla^2 H_i. \tag{12}
\]

From (8) and (9) and the condition that \( T=T_o \) far upstream, \( H_i \) can be expressed as a linear function of \( Z \) as \( H_i=A_i+B_i Z \) where \( A_i \) and \( B_i \) are constants determine from the conditions \( Y_F=1 \) in fuel stream and \( Y_F=0 \) in oxidizer stream. Thus, using the definition of \( H_i \), the reactants mass fractions, \( Y_F \) and \( Y_X \), may be expressed in terms of \( Z \) and \( T \) as follows:

\[
Y_F = (T_o-T) \frac{m_F v_F c_p}{Q} + Z \tag{13}
\]

\[
Y_X = (T_o-T) \frac{m_X v_X c_p}{Q} - Z + 1 \tag{14}
\]

B. Dimensionless Variables

In order to express the basic equations in terms of dimensionless variables, we identify suitable dimensionless parameters so that the magnitude of the parameters will be of order unity. Thus, we introduce the dimensionless density \( \sigma = \rho/\rho_o \) and dimensionless velocity \( (U,V)=(\mathbf{u}/U_o,v/U_o) \) as well as dimensionless coordinates \( (X,Y)=(x/U_o,y/U_o) \). The maximum temperature is reached just behind the flame front along the stoichiometric line, where the combustion is complete and neither fuel nor oxidizer left in the product stream. We obtain this 'Adiabatic Flame Temperature', \( T_s \), by putting \( Z=Z_s=1/(1+r) \) and \( Y_F=0 \) in (13)

\[
T_s = T_o + \frac{Q}{m_F v_o c_p} \frac{1}{1+r} = T_o + \frac{Q}{(m_F v_o + m_X v_o) c_p}. \tag{15}
\]
The dimensionless parameter \( \alpha \) characterizes the temperature rise, or amount of heat released in the flame:

\[
\alpha = \frac{T_r - T_{\infty}}{T_r} = \left[ 1 + \frac{(m_x v_x + m_y v_y) c_p T_r}{Q} \right]^{-1}.
\]  

(16)

Further, we will introduce dimensionless temperature, \( \Theta \), as well as the Zeldovich number, \( \beta \), defined as

\[
\Theta = \frac{T - T_{\infty}}{T_r - T_{\infty}},
\]

(17)

\[
\beta \equiv \frac{T_r}{T_{\infty}}.
\]

(18)

In terms of dimensionless variables, (6) may be written as

\[
\sigma(U \frac{\partial \Theta}{\partial x} + V \frac{\partial \Theta}{\partial y}) = \frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2}
\]

\[
+ \beta \sigma (1 - \Theta) \exp \left[ -\frac{\beta(1-\Theta)}{1(1-\Theta)} \right] \gamma \Theta^* \cdot Q.
\]

(19)

Where \( \Sigma \) is defined by

\[
\Sigma(x, y) = (x - y)^{\nu} \left[ (1 - x) + r(1 - y) \right]^{\nu_x}.
\]

(20)

And \( \lambda \) and \( \gamma \) are defined by

\[
\lambda = \frac{kQ4}{c_p T_r \alpha (1 + r) v_y v_x} \exp(-\beta / \alpha) \frac{1}{U_{\infty}},
\]

(21)

\[
\gamma = \frac{Bn (4 \pi^2)}{c_p m_x v_x c_p} \left( \frac{QZ}{m_x c_p} \right)^{n_x}
\]

(22)

In terms of dimensionless variables, the equation for mixture fraction, \( Y \), equation (5) becomes

\[
\sigma \left( U \frac{\partial Z}{\partial x} + V \frac{\partial Z}{\partial y} \right) = \frac{\partial^2 Z}{\partial x^2} + \frac{\partial^2 Z}{\partial y^2}
\]

(23)

The dimensionless boundary conditions become \( \Theta(-1, y) = 0; \Theta(0, y) = 1 \); and \( \Theta(y, 0) = 0 \).

In order to obtain analytical solution, we introduce some approximation in which \( \sigma \) may be taken unity. Also \( U = 1 \) and \( V = 0 \). Therefore, (19) and (23) respectively become

\[
\frac{\partial \Theta}{\partial x} = \frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2}
\]

(24)

\[
+ \lambda \sigma (Z / Z_r, \Theta) \exp \left[ -\beta(1-\Theta) \right] \gamma \Theta^* \cdot Q.
\]

(25)

III. ACTIVATION ENERGY ASYMPTOTIC

Zeldovich number \( \beta \) defined by (18) is considered large for many practical processes. Thus we study the basic dimensionless equations describing flames in the asymptotic limit of \( \beta \rightarrow \infty \). This limit is known as Activation Energy Asymptotic (AEA). It is clear from (24) that the source term vanishes and becomes

\[
\frac{\partial \Theta}{\partial x} = \frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} - \Theta
\]

(26)

Equation (26) is a linear homogeneous partial differential equation which is converted to Helmholtz differential equation by changing the variable \( \Theta \) to \( \psi \) by the substitution

\[
\Theta(X, Y) = \exp \left( \frac{1}{2} X \right) \psi(X, Y)
\]

(27)

So, (26) becomes

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} - \frac{5}{4} \psi = 0
\]

(28)

Equation (28) is a two-dimensional homogeneous Helmholtz equation in the rectangular Cartesian system of coordinates which may be solved by separation of variables method. The boundary conditions also become \( \psi(-1, y) = 0; \psi(0, y) = 1 \); and \( \psi(y, 0) = 0 \).

\[
\psi = \sum_{n} \frac{2 \sin(k_n L)}{k_n} e^{\frac{k_n^2 \beta^2}{1 - \epsilon^{(2k_n^2/5)} X}} e^{\frac{k_n^2 \beta^2}{1 - \epsilon^{(2k_n^2/5)} X}} \cos k_n Y
\]

(29)

From (27) the triple flame temperature is obtained

\[
\Theta = \sum_{n} \frac{1}{k_n} \sum_{n} \frac{2 \sin(k_n L)}{k_n} e^{\frac{k_n^2 \beta^2}{1 - \epsilon^{(2k_n^2/5)} X}} e^{\frac{k_n^2 \beta^2}{1 - \epsilon^{(2k_n^2/5)} X}} \cos k_n Y
\]

(30)
IV. CONCLUSIONS

Here, we may present some results for variations of the dimensionless flame temperature versus the dimensionless coordinates. (Fig.1)

Besides, the dimensionless temperature along X-axis and Y-axis are shown in Fig.(2) and Fig.(3) respectively. As can be seen in Fig.(2), the rate of variation of $\Theta$ versus Y is increased by increase in X. It means that the temperature will increase by moving along X-axis.

It can be seen from Fig.(2) that the flame temperature has an increasing trend along X-axis. While Y increases from 0 to 50, the flame temperature slightly decreases along x-axis. Fig.(3) demonstrates that the flame temperature versus the coordinate Y will increase while X increases from 0 to 1.

The flame temperature trend has good agreement with numerical works.

The increasing interest in the study of the triple flame is due to its unique propagation behavior in fuel/air mixing layers as well as flame stabilization in laminar and turbulent jets. The analytical studies and experiments have several limitations. In this paper we consider the fuel containing volatile particle such as Lycopodium and study the effects of vaporization term on the temperature distribution.

V. REFERENCES